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Asymptotic Expansions for the Joint and Marginal Distributions of the Latent Roots of the Covariance Matrix

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1. Introduction.

Let nS be an $m \times m$ matrix having the Wishart distribution $W_m(n, \Sigma)$. Let $l_1 > l_2 > \dots > l_m > 0$ and $\lambda_1 > \lambda_2 > \dots > \lambda_m > 0$ denote the latent roots of S and Σ respectively. For large n and simple latent roots of Σ , it is known that the latent roots of S are asymptotically independently normal. We assume throughout this paper that all the roots of Σ are simple. In this paper an expansion, up to and including the term of order n^{-1} , is given for the joint density function of l_1, \dots, l_m in terms of normal density functions. Expansions for the marginal distributions of the roots are also given, valid when the corresponding roots of Σ are simple.

2. Expansions for the extreme root distributions.

We consider first the largest root l_1 . From the exact

expression for the distribution function of l , by Sugiyama [15], [16], the distribution function of $\chi_i = (n/2)^{1/2} (l_i / \lambda_i - 1)$ can be written as

$$(2.1) \quad P(\chi_i < x) = [\Gamma_m(p) / \Gamma_m(\frac{1}{2}n + p)] (\det R)^{n/2} {}_1F_1(\frac{1}{2}n; \frac{1}{2}n + p; -R),$$

where $p = \frac{1}{2}(m+1)$, $\Gamma_m(a) = \pi^{m(m-1)/4} \prod_{i=1}^m \Gamma(a - (i-1)/2)$, $R =$

$\text{diag}(\gamma_1, \gamma_2, \dots, \gamma_m)$ with $\gamma_i = \{n/2 + (n/2)^{1/2} x\} z_i$, $z_i = \lambda_i / \lambda_i$

($i=1, \dots, m$) and ${}_1F_1$ is a confluent hypergeometric function of matrix argument (see Herz [7], Constantine [5]). A system of partial differential equations (pde's) satisfied by the ${}_1F_1$ function has been given by Muirhead [12]. Starting with this system it can be readily verified that $P \equiv P(\chi_i < x)$ satisfies each of the m pde's

$$(2.2) \quad \frac{\partial^2 P}{\partial x^2} + x \frac{\partial P}{\partial x} + \left(\frac{2}{n}\right)^{\frac{1}{2}} \left[2x \frac{\partial^2 P}{\partial x^2} + \left(1 + x^2 - \frac{1}{2} A_1\right) \frac{\partial P}{\partial x} - x \sum_{k=2}^m z_k \frac{\partial P}{\partial z_k} - 2 \sum_{k=2}^m z_k \frac{\partial^2 P}{\partial x \partial z_k} \right] + \frac{2}{n} \left[x^2 \frac{\partial^2 P}{\partial x^2} + x \left(1 - \frac{1}{2} A_1\right) \frac{\partial P}{\partial x} + \sum_{k=2}^m z_k \left(1 + \frac{1}{2} A_1 - \frac{1}{2(1-z_k)}\right) \frac{\partial P}{\partial z_k} - 2x \sum_{k=2}^m z_k \frac{\partial^2 P}{\partial x \partial z_k} + \sum_{k=2}^m \sum_{j=2}^m z_j z_k \frac{\partial^2 P}{\partial z_k \partial z_j} \right] = 0$$

and

$$(2.3) \quad (z_i - 1) \frac{\partial P}{\partial z_i} + \left(\frac{2}{n}\right)^{\frac{1}{2}} \left[\frac{1}{2(1-z_i)} \frac{\partial P}{\partial x} + x z_i \frac{\partial P}{\partial z_i} \right] + \frac{2}{n} \left[z_i \frac{\partial^2 P}{\partial z_i^2} \right]$$

$$\begin{aligned}
& + \frac{x}{2(1-z_i)} \frac{\partial P}{\partial x} + (1 - \frac{1}{2} A_i) \frac{\partial P}{\partial z_i} - \frac{1}{2(1-z_i)} \sum_{k=2}^m z_k \frac{\partial P}{\partial z_k} \\
& - \frac{1}{2} \sum_{\substack{j=2 \\ j \neq i}}^m \frac{z_j}{z_i - z_j} \frac{\partial P}{\partial z_j}] = 0 \quad (i=2, 3, \dots, m),
\end{aligned}$$

where

$$(2.4) \quad A_i = \sum_{\substack{j=1 \\ j \neq i}}^m \frac{z_i}{z_j - z_i} \quad (i=1, 2, \dots, m).$$

We now look for a solution of these m p.d.e's (2.2)

and (2.3) of the form

$$(2.5) \quad P = \Phi(x) + \sum_{k=1}^{\infty} (2/n)^{k/2} Q_k,$$

where the Q_k are functions of x, z_2, \dots, z_m . (That P possesses such an expansion follows from results in the next section.)

We substitute the series (2.5) into (2.2) and (2.3) and equate coefficients of powers of $(2/n)^{1/2}$ on the L.H.S.'s to zero. Equating the coefficient of $(2/n)^{1/2}$ in (2.2) and (2.3) to zero and using the boundary conditions $P(x, < \infty) = 1$ and $P(x, < -\infty) = 0$, we have

$$(2.6) \quad Q_1 = -(1/6) \Phi(x) [2H_2(x) + 3A_1 H_0(x)],$$

where $H_j(x)$ denotes the Hermite polynomial of degree j (see Kendall and Stuart [9], p. 155). Similarly, equating the coefficient of $2/n$ in (2.2) and (2.3) to zero and solving

the resulting equations gives

$$(2.7) \quad Q_2 = -(1/72) \mathcal{G}(x) [4H_2(x) + 18H_3(x) + 12A_1H_3(x) - 18B_1H_1(x) + 9A_1^2H_1(x)],$$

$$\text{where } A_1 = \sum_{j=2}^m (z_j - 1)^{-1}, \quad B_1 = \sum_{j=2}^m (z_j - 1)^{-2}.$$

Coefficients of higher powers of $(2/n)^{1/2}$ in (2.5) may be obtained in a similar manner if required. The expansion is summarized in the following

Theorem 2.1. The distribution function of $x_1 = (n/2)^{1/2} (l_1/\lambda_1 - 1)$, when the latent roots of Σ are simple, can be expanded for large n as

$$(2.8) \quad P(x_1 < x) = \Phi(x) + (2/n)^{1/2} Q_1 + (2/n) Q_2 + O(n^{-3/2}),$$

where Q_1 and Q_2 are given by (2.6) and (2.7) respectively.

Consider now the distribution of the smallest root l_m .

Since nS is $W_m(n, \Sigma)$ we have

$$(2.9) \quad P(l_m > y) = \left[\left(\frac{1}{2}n \right)^{\frac{1}{2}mn} (\det)^{-\frac{1}{2}n} / \Gamma_m\left(\frac{1}{2}n\right) \right] \int_{S > yI} \exp\left(-\frac{1}{2}n \operatorname{tr}(\bar{\Sigma}^{-1}S)\right) \det S^{\frac{1}{2}n-p} dS.$$

Making the transformation $T = y^{-1}S - I$ it is easily seen that

(2.9) becomes

$$(2.10) \quad P(l_m > y) = \left[\Gamma_m(p) / \Gamma_m\left(\frac{1}{2}n\right) \right] \det\left(\frac{1}{2}ny \bar{\Sigma}^{-1}\right)^{\frac{1}{2}n} \exp\left(-\frac{1}{2}ny \operatorname{tr} \bar{\Sigma}^{-1}\right) \cdot \Psi\left(p, \frac{1}{2}n+p; \frac{1}{2}ny \bar{\Sigma}^{-1}\right),$$

where $\Psi(a, c; R) \stackrel{\text{def.}}{=} \left\{ 1/\prod_m (a) \right\} \int_{S>0} \exp(-\text{tr}(RS)) (\det)^{a-p} \det(I+S)^{c-a-p} dS.$

The function Ψ is another confluent hypergeometric function of matrix argument (see Muirhead [13]).

Putting $x_m = (n/2)^{1/2} (l_m / \lambda_m - 1)$ and using the system of pde's satisfied by the Ψ function given by Muirhead [13] it can readily be shown that the distribution function of x_m , $P \equiv P(x_m < x)$, satisfies each of the m pde's (2.2) and (2.3). The only difference here is that now $z_i = \lambda_m / \lambda_{m-i+1}$ instead of λ_1 / λ_i as it was in the largest root distribution. Hence

Theorem 2.2. The distribution function of $x_m = (n/2)^{1/2} (l_m / \lambda_m - 1)$, when the latent roots of Σ are simple, can be expanded for large n as

$$P(x_m < x) = \Phi(x) + (2/n)^{1/2} Q_1 + (2/n) Q_2 + O(n^{-3/2}),$$

where $z_i = \lambda_m / \lambda_{m-i+1}$ in Q_1 and Q_2 given by (2.6) and (2.7) respectively.

3. Expansion for the joint distribution.

The joint density function of l_1, \dots, l_m can be

expressed in the form (see James [8])

$$(3.1) \quad \pi^{\frac{1}{2}m^2} (\frac{1}{2}n)^{\frac{1}{2}mn} [\Gamma_m(\frac{1}{2}n) \Gamma_m(\frac{1}{2}m)]^{-1} \prod_{i=1}^m l_i^{\frac{1}{2}n-p} \lambda_i^{-\frac{1}{2}n} \prod_{i,j=1}^m (l_i - l_j) {}_0F_0(-\frac{1}{2}nL, \Sigma^{-1}),$$

where $p = \frac{1}{2}(m+1)$, $L = \text{diag}(l_1, \dots, l_m)$, $\Sigma = \text{diag}(\lambda_1, \dots, \lambda_m)$ and ${}_0F_0$ is a hypergeometric function with two argument matrices. The ${}_0F_0$ function in (3.1) has been expanded for large n by G. Anderson [1] by expressing it as an integral over the orthogonal group. In [1] it is shown that the joint density function can be expressed as

$$(3.2) \quad k_1 \prod_{i=1}^m [\lambda_i^{(m-n-1)/2} l_i^{n/2-p} \exp(-nl_i/2\lambda_i)] \prod_{i,j=1}^m [(l_i - l_j)/(l_i - \lambda_j)]^{1/2} \cdot G,$$

where $k_1 = (n/2)^{mn/2 - m(m-1)/4} / \prod_{i=1}^m \Gamma((n-i+1)/2)$

and

$$(3.3) \quad G = 1 + (2n)^{-1} \sum_{i,j=1}^m \lambda_i \lambda_j (\lambda_i - \lambda_j)^{-1} (l_i - l_j)^{-1} + O(n^{-2}).$$

(Anderson did not show in general that the remainder term in (3.3) is of order n^{-2} ; this has been shown by the author in her Ph.D. thesis at Yale University in the more general case.) Now putting $x_i = (n/2)^{1/2} (l_i / \lambda_i - 1)$ ($i=1, \dots, m$), from (3.2) the joint density function of x_1, \dots, x_m can be expressed as

$$(3.4) \quad k_2 F_1 F_2 \left\{ 1 + (2n)^{-1} \sum_{i,j}^m \lambda_i \lambda_j / (\lambda_i - \lambda_j)^2 + O(n^{-3/2}) \right\},$$

where

$$k_2 = (n/2)^{mn/2 - m(m+1)/4} \exp(-mn/2) / \prod_{i=1}^m \Gamma((n-i+1)/2),$$

$$F_1 = \prod_{i=1}^m \left\{ \left(1 + \left(\frac{2}{n} \right)^{1/2} x_i \right)^{n/2 - 1} \exp \left(- \left(n/2 \right)^{1/2} x_i \right) \right\}$$

and

$$F_2 = \prod_{i,j}^m \left\{ 1 + \left(\frac{2}{n} \right)^{1/2} (x_i \lambda_i - x_j \lambda_j) / (\lambda_i - \lambda_j) \right\}^{1/2}.$$

It remains to expand k_2 , F_1 and F_2 in (3.4) for large n . For example, by expanding the gamma functions for large n it follows that

$$k_2 = (2\pi)^{-m/2} \left[1 - (24n)^{-1} m(2m^2 + 3m - 1) + O(n^{-2}) \right].$$

The functions F_1 and F_2 can be easily expanded in terms of powers of $n^{-1/2}$; however these expansions, up to and including the terms of order n^{-1} , are quite lengthy and are omitted here. Substituting these expansions in (3.4) gives an expansion of the joint density function of x_1, \dots, x_m .

The final result is summarized in the following

Theorem 3.1. The joint density function of $x_i = (n/2)^{1/2} (\lambda_i / \lambda_i - 1)$ ($i=1, \dots, m$), where $\lambda_1, \dots, \lambda_m$ are simple roots of Σ , may be expanded for large n as

$$(3.5) \quad \prod_{i=1}^m \varphi(x_i) \cdot \left\{ 1 + (2/n)^{1/2} \sum_{i=1}^m P_{1i}(x_i) + (2/n) \left(\sum_{i=1}^m P_{2i}(x_i) + \sum_{i,j}^m P_{1i}(x_i) P_{1j}(x_j) + \frac{1}{2} \sum_{i,j}^m \frac{x_i x_j \lambda_i \lambda_j}{(\lambda_i - \lambda_j)^2} \right) + O(n^{-3/2}) \right\},$$

where

$$(3.6) \quad P_{1i}(x) = (1/6) \{ 2H_3(x) + 3A_i H_1(x) \},$$

$$(3.7) \quad P_{2i}(x) = (1/72) \{ 4H_6(x) + 18H_4(x) + 12A_i H_4(x) - 18B_i H_2(x) + 9A_i^2 H_2(x) \},$$

$H_j(x)$ is the Hermite polynomial of degree j , and

$$(3.8) \quad A_i = \sum_{\substack{j=1 \\ j \neq i}}^m \lambda_j / (\lambda_i - \lambda_j), \quad B_i = \sum_{\substack{j=1 \\ j \neq i}}^m \lambda_j^2 / (\lambda_i - \lambda_j)^2.$$

Note that A_i is the same as in (2.4).

By integrating out the other variables in (3.5) an expansion of the marginal density function of x_i can be obtained.

Corollary The marginal density function of $x_i = (n/2)^{1/2} (\lambda_i / \lambda_i - 1)$, where λ_i is a simple root of Z , may be expanded for large n as

$$(3.9) \quad \varphi(x_i) \{ 1 + (2/n)^{1/2} P_{1i}(x_i) + (2/n) P_{2i}(x_i) + O(n^{-3/2}) \},$$

where $P_{1i}(x_i)$ and $P_{2i}(x_i)$ are given by (3.6) and (3.7) respectively.

The expansion (3.9), in the cases $i=1$ and n , agrees with the expansions for the extreme root distributions given in the previous section. Sugiura [14] has also obtained (3.9) using another method.

Asymptotic moments of l_i can be obtained from (3.9); we obtain

$$E(l_i) = \lambda_i + A_i \lambda_i / n + O(n^{-2}),$$

$$(3.10) \quad \text{Var}(l_i) = 2\lambda_i^2 / n - 2\lambda_i^2 B_i / n^2 + O(n^{-3}),$$

$$\kappa_3(l_i) = 8\lambda_i^3 / n^2 + O(n^{-3}), \quad \kappa_4(l_i) = 48\lambda_i^4 / n^3 + O(n^{-4}),$$

where $\kappa_3(l_i)$ and $\kappa_4(l_i)$ denote the third and fourth cumulants of l_i and A_i, B_i are given by (3.8).

From (3.5) we obtain

$$(3.11) \quad \text{Cov}(l_i, l_j) = 2 \left[\lambda_i \lambda_j / (\lambda_i - \lambda_j) \right]^2 / n^2 + O(n^{-3}).$$

These expansions agree with results obtained by Lawley [11] without using the asymptotic normality.

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